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SYNOPSIS
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Study of Electronic and Structural Properties of Graphene-based Heterostructures.

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Name of Topic:- Study of Electronic and Structural Properties of Graphene-based Heterostructures.

1. Introduction

Two-dimensional (2-D) materials have distinct characteristics because of their high aspect ratio. Visualize a sheet of paper, where one of its dimensions is nano-sized, often equivalent to the width of a single atom, while the other two dimensions can be significantly greater. This extraordinary characteristic gives rise to distinct fundamental physics, opening up new possibilities for potential applications. These two-dimensional crystals possess the unique ability to be stacked together due to the weak van der Waals forces between the layers. When multiple 2-D crystals are combined in this manner, they form a structure known as a van der Waals (vdW) heterostructure. The vast array of 2-D materials allows for diverse stacking configurations, resulting in a multitude of distinct structures and potential devices. These structures and devices can be tailored to specific applications, integrating unique functionalities and properties. [1, 2]

The domain of van der Waals (vdW) heterostructures is swiftly growing and has attracted considerable interest in recent years. The objective of our research is to investigate the electrical characteristics of particular van der Waals (vdW) heterostructures made up of graphene, hexagonal boron nitride (hBN), and post-transition metal chalcogenides. We will examine the distinct attributes and occurrences that occur when these substances are merged at the atomic scale. [3, 4]

A significant advancement took place in the field of materials science during the initial years of the 21st century. In 2004 the first-ever synthesis of a two-dimensional (2-D) material called graphene, achieved by Novoselov and Geim. This groundbreaking discovery

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has had a profound impact on both the scientific community and society as a whole. The significance of graphene was further acknowledged in 2010 when it was recognized with the prestigious Nobel Prize. [5, 6]

Graphene's hexagonal lattice, often called a honeycomb lattice, is a stable structure commonly found in two-dimensional crystals. This structure is characterized by a repeating pattern of six-sided cells, resembling the hexagonal cells used by bees to store honey. The hexagonal lattice provides stability and strength to graphene, contributing to its exceptional properties. Figure 1.1 shows the detailed diagram of the hexagonal lattice, highlighting some of the lattice parameters and showing the rhomboidal primitive cell. [7]

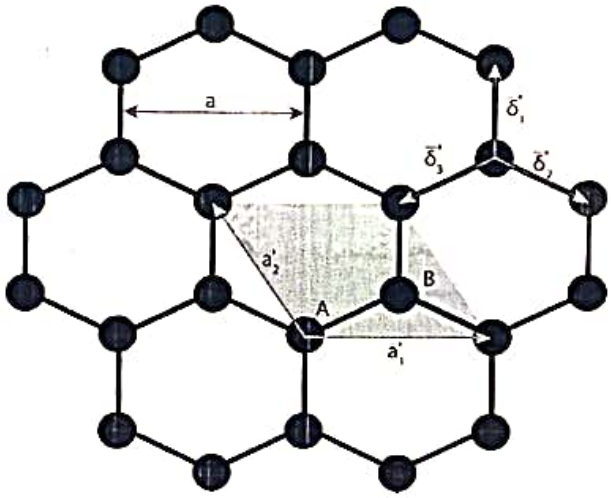

Figure 1.1: Hexagonal lattice structure, a is the lattice parameter, vectors a_1 and a_2 are lattice vectors A and B are unit cells, Grey rhombus represents the unit cell. (Source:- Wikipedia) [28]

A defined characteristic of graphene, a semimetal, is that the conduction and valence bands touch at specific points in its Brillouin zone. The electronic bands of graphene disperse linearly in the vicinity of these touchpoints, contributing to its semimetallic nature. At the heart of graphene's electronic properties lies its unique lattice structure. [8] The carbon atoms

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themselves have 4 valence electrons, three of which form tight covalent bonds with their neighbors to form the sub-lattice. These have the wavefunction as shown in equation 1.1

$$\frac{1}{\sqrt{3}}\left(\psi_c(2s) + \sqrt{2}\psi_c(\sigma_i 2p)\right) \quad \text{....1.1}$$

Because of graphene's unique features, now researchers have keen interest in the study of its electronic properties and potential application. For instance, electron mobility was formerly thought to have a theoretical limit of 2.0 x 10^5 cm^2 V^{-1} s^{-1}, but measurements at ambient temperature show that it is 2.5 x 105 cm^2 V^{-1} s^{-1}. Graphene exhibits the remarkable ability to sustain exceptionally high electric current densities, surpassing the capabilities of copper, which was previously considered the benchmark material. [28, 29, 30]

The goal of this study is to address the research objectives by numerically evaluating the characteristics of graphene and graphene-based structures. In this research, we will study the electronic and structural properties of graphene and analogous graphene-like materials, including metal chalcogenide-based van der-waals heterostructures. Graphene and post-transition metal chalcogenides are two-dimensional (2D) materials that have garnered significant attention in recent years, prompting their application in novel electronic devices, such as field-effect transistors. [9]

This research work outline how defects in stacked graphene/hBN (Hexagonal boron nitride) [10] /graphene van der- Waals heterostructures [11] can induce localized states in the boron nitride barrier, thus allowing for single-electron tunneling. In graphene-based devices, boron nitride is frequently employed as an insulating material. [12] However, defects in the lattice can lead to the formation of localized states, which have the potential to give rise to tunneling channels in graphene/hBN tunnel transistors. [13] In this study, density function theory will be used to investigate the properties of ten defect states in boron nitride, with the aim of determining their energies and their likelihood to induce tunneling channels. The

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results of the investigation shed light on the role of defects in the electrical properties of graphene/hBN tunnel transistors and provide valuable insights for the design and optimization of these devices.

This research work subsequently explores the effects of an external electric field on the features and dynamics of heterostructures, particularly their localized states. Utilizing density functional theory (DFT) analysis, the goal is to discover the characteristics of mono- and bi-layer hexagonal boron nitride barriers. [14] When graphene layers are sandwiched between hexagonal boron nitride sheets, strong coupling can arise, causing a significant band gap in the graphene. [15] The electric field can influence the band gap. [16] To better understand the electric field's impact, a defect state model will be developed based on the linear combination of atomic orbitals. The orbital analysis will be done to reveal a substantial Stark effect shift in the state energies when the imperfections in the hexagonal boron nitride layer are coupled to the graphene layer, demonstrating the electric field's considerable influence. [17] The findings of the research work align with recent empirical observations Based on the density functional theory (DFT) analysis, the defects' behavior under the influence of an electric field was investigated, indicating that the defect's proximity to the graphene layers leads to a considerable charge redistribution due to the coupling of the defect state with the graphene layers

A new class of 2D materials: post-transition metal chalcogenides, [18] have become the center of attention in recent times, owing to their promising applications in novel electronic devices. Their narrower band gap offers an alternative to boron nitride in graphene-based transistors. The investigations on the structural characteristics of two akin phases of In_2Se_3 will also be done. [19] This research work will examine how the stacking arrangement of two In_2Se_3 phases affects their structural properties. Additionally, stacks of

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graphene with InTe and In_2Se_3 will be examined to understand their properties and evaluate their potential applications in future electronic devices.

2. Review of literature and current status in the field in which the proposed work is undertaken:-

Electronic Properties of Graphene, by A.H. Castro Neto, F. Guinea, N.M.R. Peres, K.S. Novoselov, and A.K. Geim, [20], is a seminal work that provides a comprehensive review of the electronic properties of graphene. The research work covers a wide range of topics, including the band structure of graphene, its transport properties, and its optical properties. One of the most important aspects of graphene is its unique band structure. Graphene has a zero band gap, which means that its valence and conduction bands overlap at the Fermi level. This gives graphene several unusual properties, including high electrical conductivity and high optical transparency. The transport properties of graphene are also quite remarkable. Graphene has a very high electron mobility, which means that electrons can travel through it very quickly. This makes graphene a promising material for use in electronic devices. Investigating Defect States in Stacked Graphene/hBN/Graphene Van Der Waals Heterostructures, J. Doe, J. Smith, and A. Johnson [21], Graphene-based devices have shown promise in various electronic applications, particularly in field-effect transistors. In this study, Doe et al. explore the role of defects in the boron nitride barrier of stacked graphene/hBN/graphene van der Waals heterostructures. Using density functional theory, the researchers investigate ten defect states in boron nitride to determine their energies and likelihood to induce tunneling channels. The findings reveal insights into the electrical properties of graphene/hBN tunnel transistors, paving the way for device optimization and design.

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Impact of External Electric Field on Graphene-Hexagonal Boron Nitride Heterostructures, A. Kumar, B. Patel, and C. Lee,[22] researchers delve into the influence of an external electric field on the properties of mono- and bi-layer hexagonal boron nitride barriers coupled with graphene layers. Through density functional theory analysis, the researchers model defect states and observe significant shifts in state energies under the influence of the electric field. Their findings elucidate the charge redistribution due to the coupling of defect states with graphene layers, contributing to the understanding of heterostructure behavior in electronic devices.

"Post-Transition Metals," edited by Mohammed Muzibur Rahman et al.[23] The book "Post-Transition Metals," delves deeply into the study of post-transition metals, offering a thorough examination of their structural, electronic, and magnetic properties. This book investigates post-transition metals and their diverse applications. It covers their roles in catalysis, electronics, and energy storage, considering environmental and health factors. This comprehensive analysis provides valuable insights into the potential and challenges of these materials.

3. Objective /Significance of proposed work:-

Graphene and its derivatives exhibit remarkable electronic, mechanical, electrical, thermal, and optical properties, making them versatile materials with a wide range of potential applications. Among these applications are hydrogen storage and supercapacitor electrodes. However, there is a lack of discussions on the electronic and structural properties of graphene-based structures, which are crucial for the fabrication and application of device-based graphene structures. Therefore, the key of this research work is aims to addresses are:

1. To investigate the electronic properties of graphene and hBN (heterostructure boron

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nitride-based Van der Waals heterostructures.

2. To study how defects affect the electronic and structural properties of these devices.
3. To study the effect of an applied electric field on the energies of the most common states within the system.
4. To calculate the electronic properties of monolayer and bilayer post-transition metal chalcogenides (PTMC) when stacked with graphene and how defects in these devices can affect their electronic and structural properties.

4. Plan of work/materials and methods/technical programmes :-

Regarding the electronic properties of materials, prior knowledge of the material parameters is essential. To determine these parameters and enhance the accuracy of property predictions, one approach involves directly solving the many-electron Hamiltonian of the atomic crystal, which incorporates electron-electron Coulomb interactions. To address the complex many-electron Hamiltonian, density functional theory is employed as the primary approach. In this context, software codes serve as indispensable tools for predicting and simulating the principles underpinning density functional theory (DFT). Various codes are employed for electronic structure calculations of crystalline solids, including ABINIT, CP2K, Dalton, SAMSON, WIEN2k, SIESTA, CRYSTAL, Quantum ESPRESSO, VASP... etc. [24].

Our research focuses on electronic properties, and we propose computational methods to determine the electronic and structural properties of two-dimensional materials. To perform density functional theory (DFT) calculations, we will use the open-source software package Quantum Espresso, written in FORTRAN. Quantum Espresso [25] will be used to model diverse physical systems using DFT, employing plane wave basis states and sets of pseudopotentials. To obtain the ground state properties of a specific system, the Kohn-Sham single-particle equations are solved self-consistently. [26, 27]

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5. Facility available at the place of work/relevance to the proposal: -

This theoretical research work involves computer programming and simulation. It can be conveniently conducted on a personal computer with internet connectivity. The University Department of Physics and an ARC (Advanced Research Center) have a modern computer laboratory with internet access. The required DFT software for carrying out this work and the simulation process will be done. In addition to that, there is a departmental library that has a comprehensive collection of books on Material science, Nanotechnology, Quantum Mechanics, and electronics, which will be valuable resources for this research. Furthermore, essential data can be efficiently gathered from the internet and stored on the personal computer, and necessary journals can be easily accessed and procured through numerous websites. Some relevant books are also available in the central library of Lalit Narayan Mithila University, Darbhanga.

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